A Home for Energetic Materials

Livermore's Energetic Materials Center is advancing scientific understanding of high explosives.

and Their Experts

FOR centuries, militaries have tapped the extraordinary energy locked in the molecules of energetic materials: shock waves with speeds approaching 10 kilometers per second, pressures up to 500,000 times that of Earth's atmosphere, rapidly expanding gases reaching temperatures of 4,000 kelvins, and 20 billion watts of power per square centimeter of detonation front. Since Lawrence Livermore's inception in 1952, Laboratory researchers have been among the nation's leaders in understanding, synthesizing, formulating, testing, and modeling the chemical high explosives (HE) that are an integral part of every nuclear weapon system. Such violent reactions were once extremely difficult to accurately predict, characterize, and control. However, scientific understanding of these physical and chemical phenomena has progressed significantly during the last few decades.

Since its founding in 1991, Livermore's Energetic Materials Center (EMC) has been the focal point for research and development of explosives, propellants, and pyrotechnics at the Laboratory. EMC provides oversight and direction for HE efforts at Livermore, ensuring full advantage is taken of Laboratory-wide capabilities. In 2008, the National Nuclear Security Administration (NNSA) named Livermore its HE R&D Center of Excellence because of EMC and the people and research facilities that support it. The center is located at the High Explosives Applications Facility (HEAF), where the majority of high-explosives synthesis, formulation, experiment, and theory are performed at Livermore.

Explosives, such as the well-known trinitrotoluene (TNT), react in millionths of a second, and their high-power properties are used in a variety of warheads and bombs. Propellants release similar amounts of chemical energy as explosives but over a longer period (seconds). The gases they generate are thus useful in launching objects such as artillery shells or rockets. In contrast, pyrotechnics generate only heat and light and are used to weld and cut. Pyrotechnics are more commonly found in fireworks. EMC provides expertise on all three types of energetic materials to the Department of Energy, NNSA, Department of Defense, Department of Homeland Security, Transportation Security Administration, Federal Bureau of Investigation (FBI), and other law-enforcement and government organizations.

According to EMC Director Jon Maienschein, "We needed to strengthen collaborations and integrate all the disparate high-explosives activities, bringing them together in a facility where everything—synthesis, formulation, experiment, and theory—could be done." Scientists work on theoretical models of the behavior of energetic materials; advanced simulations to better understand the fundamental physics and chemistry of energetic materials; synthesis and formulation of new energetic molecules; experimental characterization of energetic material properties and reactions; and high-speed diagnostic instruments for measuring the chemical and physical processes that occur during a detonation. (See the box on p. 7.)

Strong Growth of Simulation

The role of computer modeling and simulation in energetic materials research has grown substantially since the founding of EMC. In Livermore simulations, linear distances may vary from a fraction of a nanometer to several meters, or more than 10 orders of magnitude. Relevant timescales also range to 10 orders of magnitude, from millionths of a second to hours. Temperatures, too, can vary widely, up to thousands of kelvins. Solving multiscale problems requires massively parallel simulation tools, such as the Laboratory's supercomputers that rank as some of the most powerful in the world.

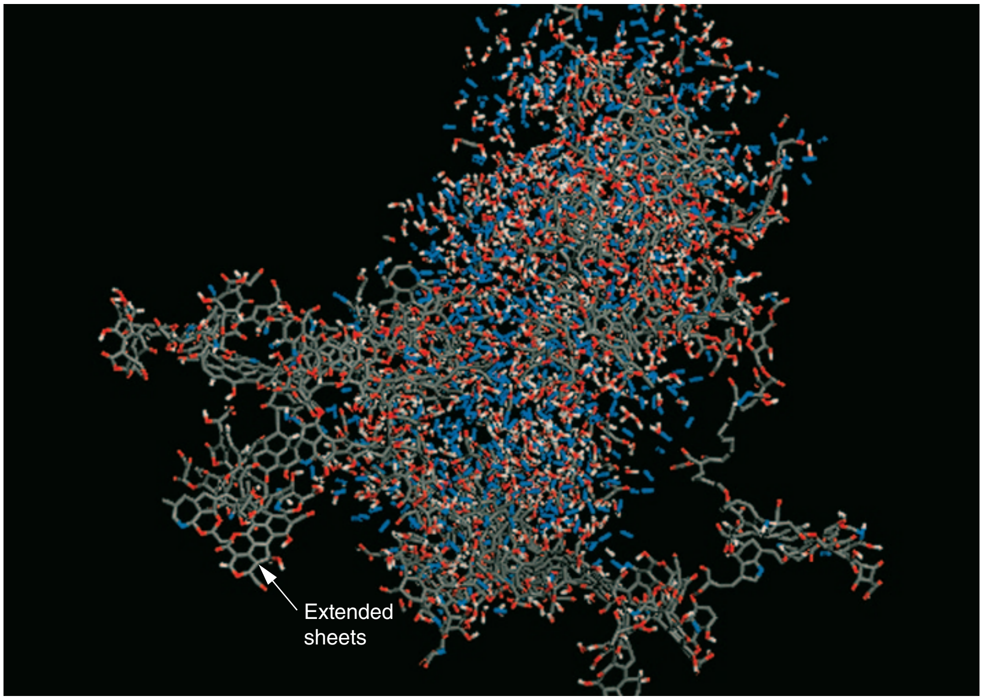
Livermore computer codes mimic the extremely rapid physical and chemical detonation processes of hundreds of energetic materials. CHEETAH is the nation's leading chemical simulation code for the performance of energetic materials, with uses ranging from nuclear weapons HE to gun propellants to improvised explosive devices (IEDs). Running on desktop computers, CHEETAH reliably runs molecular calculations based on thermodynamic properties and density parameters and converts these calculations into explosives performance measures such as detonation velocity and pressure.

The work with CHEETAH is led by computational physicist Sorin Bastea and colleagues and is based on more than a half-century of explosives experiments at Livermore. With libraries of hundreds of reactants and 6,000 products in its code, the program is used throughout the Department of Defense; version 6.0 is currently in use.

CHEETAH is linked to Livermore's hydrodynamics code ALE3D. Such a linkage, which requires hundreds of processors working in parallel, permits realistic modeling of both chemical and physical reactions across a wide envelope of detonation conditions and is invaluable in determining an explosive's safety characteristics. "ALE3D allows researchers to simulate the thermal environment of any situation," says Randy Simpson, associate program leader for Livermore's Weapons and Complex Integration Principal Directorate. "The code will track thermal expansion and chemical changes and, when an explosion finally occurs, the violence of the reaction."

Livermore codes are routinely updated to incorporate new theoretical and experimental findings. Computational physicist Larry Fried leads quantum simulations on Livermore supercomputers for NNSA's Advanced Simulation and Computing Program to strengthen the chemical and physical reaction assumptions on which CHEETAH is based. Involving thousands of microprocessors, the simulations have revealed fleeting unexpected details.

For example, simulations show that for less than 100 picoseconds, detonating high explosives act similar to a metal; that is, they become electrically conductive. Hydrogen ions become extremely mobile, while other elements remain firmly bonded to each other. In addition, simulations show that during detonation, high-explosive constituents possess characteristics of both a soup of molecules as well as a collection of high-energy ions resembling plasma. (Scientists had long debated which model was more accurate.) Finally,



A molecular dynamics simulation shows a "soup of molecules" made by detonating the high explosive 1,3,5-triamino-2,4,6-trinitrobenzene (TATB). The entire simulation is composed of more than 1 million snapshots in time. The results indicate that carbon (gray) is present in extended sheets, while nitrogen (blue), oxygen (red), and hydrogen (white) are mostly outside the sheets. This chemical insight is being incorporated into future versions of the CHEETAH code.

advanced hydrodynamics simulations using CHEETAH reveal that HE safety characteristics are highly dependent on the size of an explosive's powdered grains.

Searching for Energetic Molecules

The synthesis of new explosives with tailored properties is a cornerstone EMC activity. The work is driven by the search for molecules that yield more energy, are safer to store and handle, and are less expensive and more environmentally friendly to manufacture than current formulations. Advanced simulations make it possible to predict many material properties of new molecules, a significant improvement over the standard trial-and-error approach.

"Synthesis is both an art and a science," says chemist Phil Pagoria. For

This sequence of stop-action shots shows a bullet penetrating a sample of insensitive high explosives (IHEs) recorded at a rate of 30,000 frames per second. The bullet would have immediately detonated a more sensitive high explosives formulation on impact. The yellow cloud in the last image is unreacted IHE being expelled from the sample.

example, a chemist can attempt many multistep approaches before finding a method that produces the first few grams of a new molecule. Selecting the easiest, fastest, safest, and most environmentally friendly path requires knowledge, experience, and often the help of computer simulations. Synthesizing the first gram of an explosive may take three to six months, followed by several more months of effort to produce an optimized production process.

New molecules must pass a battery of tests that determine sensitivity to impact, friction, heat, electrostatic discharge, and shock as well as resistance to chemical decomposition. Promising molecules that pass performance and safety tests are sent to other chemists for incorporation into a mixture of ingredients, in particular binders. Additional ingredients reflect necessary trade-offs among sensitivity, performance, ease of manufacturing, safety, cost, and environmental considerations.

Synthesis and formulation chemists have helped pioneer high explosives that are remarkably insensitive to heat, shock, and impact. The most important insensitive high explosive (IHE) used in modern nuclear warheads is 1,3,5-triamino-2,4,6-trinitrobenzene (TATB), which is virtually invulnerable to significant energy release in plane crashes, fires, and explosions or to deliberate attack with small arms fire. TATB can be found in nuclear weapons, conventional munitions, and explosives used for mining and oil production. Livermore researchers developed a more

Moving beyond Nuclear Weapons

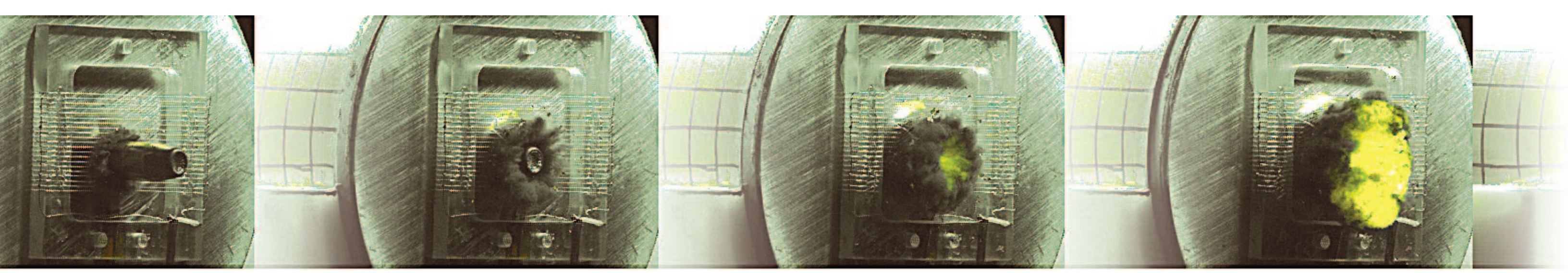
The Energetic Materials Center's (EMC's) historic emphasis has been on researching high explosives (HE) used in the main charge, booster, and detonator of a nuclear weapon's firing system. These efforts have enabled the design of and improvements to the nuclear stockpile throughout the center's history. EMC currently supports the National Nuclear Security Administration's Stockpile Stewardship Program, which ensures the safety, security, and reliability of the U.S. nuclear weapons stockpile. Toward that end, EMC researchers conduct performance and safety testing aimed at ensuring that the HE in nuclear warheads will be dependable over many decades. Routine stockpile stewardship tests examine the physical, chemical, detonation, and mechanical properties of HE taken from the nuclear stockpile.

Although HE for nuclear weapons remains a core element of scientific work, the breadth of research has grown immensely, particularly during the past decade. EMC conducts research and development for advanced conventional weapons for the Department of Defense, including new gun propellants, bombs designed to penetrate hard targets such as underground reinforced concrete bunkers, and high-speed explosive projectiles for defeating thickly armored vehicles.

As an example of new thinking for advanced conventional weapons, the Laboratory was the first to design a carbon-composite-cased munition combined with an enhanced-blast-formulation explosive. Much of the weight in today's munitions is in the steel casing. Coupled with a high explosive, the blast created by conventional steel-cased munitions can send shrapnel to distances exceeding 1 kilometer from the target, placing civilians and friendly forces at risk. Carbon-cased munitions greatly reduce collateral damage, while enabling enhanced close-in performance.

Increasingly, EMC researchers have been tasked by the Department of Defense, Department of Homeland Security, and Transportation Security Administration to investigate homemade explosives used in improvised explosive devices (IEDs) in terrorist events worldwide. This growing knowledge base includes information on detonation properties, potential safety hazards involved in their manufacture and handling, and the degree of difficulty a terrorist would face in attempting to build an IED with a particular explosive. Livermore scientists have developed an online database that includes the many explosives materials from which terrorists could build a bomb. About 1,000 federal and state scientists, engineers, and emergency responders access the database. New data are continually added as experts gain an increased understanding of terrorist capabilities and knowledge of homemade explosives.

Jon Maienschein leads the National Explosives Engineering Sciences Security Center, which applies engineering and science-based methods to assess threats and evaluate countermeasures in support of the Department of Homeland Security, Science and Technology Directorate, Explosive Division. The center is composed of scientists from Lawrence Livermore, Los Alamos, and Sandia national laboratories. One focus of the center is analyzing the vulnerability of aircraft to threats from homemade explosives. Activities include evaluating explosives formulations, including methods of initiation, detonation properties, and the probable effects on aircraft.



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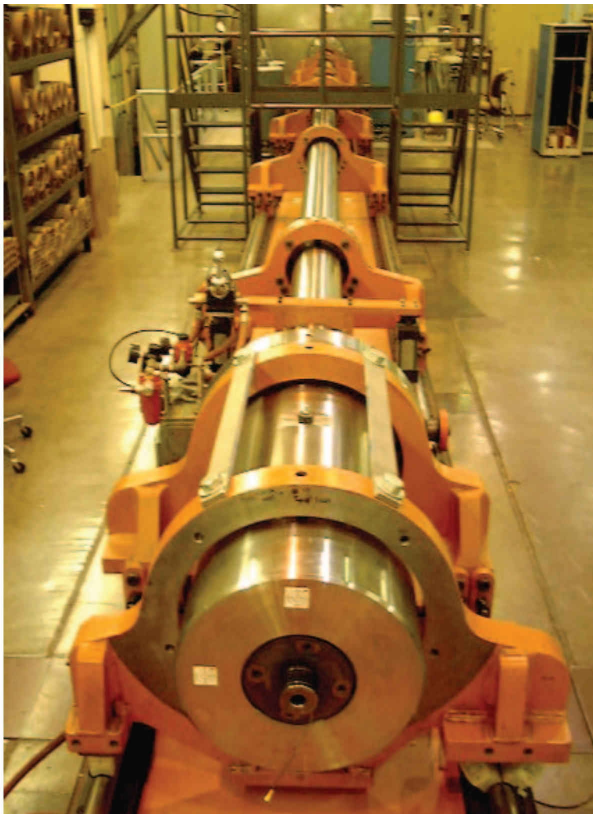

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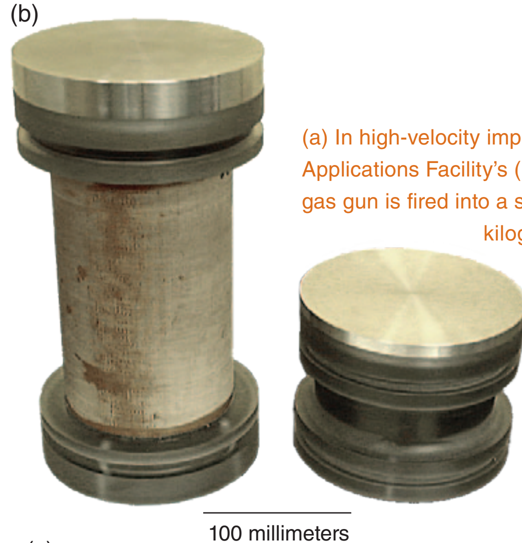

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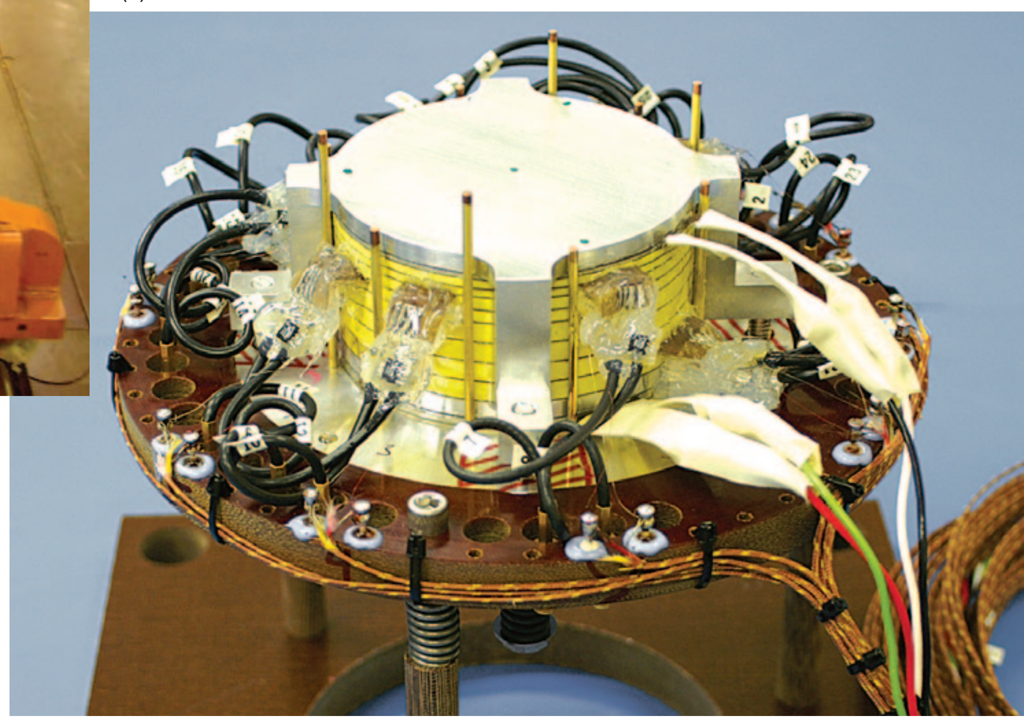


(a) In high-velocity impact studies, the High Explosives Applications Facility's (HEAF's) 100-millimeter-diameter gas gun is fired into a specially designed tank using several kilograms of propellant, with projectile velocities up to 2,500 meters per second. (b) The gun fires impactors of various sizes; smaller impactors are used for higher velocity shots. (c) The impactor hits a target composed of an outer metal layer and alternating layers of explosive (yellow) and embedded sensors.

environmentally benign and lower-cost method for producing TATB, coined the vicarious nucleophilic substitution of hydrogen method. They also developed a technique to recycle TATB crystals of superior quality from existing supplies. (See *S&TR*, June 2009, pp. 4–10.)

One IHE effort is synthesizing new molecules for use as boosters to set off the main HE charge of a nuclear device. A promising molecule is Lawrence Livermore Molecule-105 (LLM-105), which produces about 10 percent greater power than the IHE booster material ultrafine TATB. It also has greatly improved mechanical properties and performance at extreme temperatures, with safety properties similar to TATB.

For conventional munitions, LLM-172 is under development as a possible replacement material for TNT because of the latter's environmental drawbacks. LLM-172's melting point of 84°C aids processing safety because it is much lower than the temperature at which the material becomes unsafe. Livermore chemists have also developed new propellant ingredients for large guns to modify the burn rate and generate performance-improving gases. One new formulation, LLM-137, is composed of about 75 percent nitrogen, which extends the life of large gun barrels.

In addition, researchers are rethinking the very nature of new energetic materials. For example, chemist Alex Gash and materials scientist Troy Barbee are leading an effort to develop environmentally safe energetic nanolaminates that would augment or replace chemical explosives in conventional weapons. A nanolaminate is a dense solid composed of thousands of nanometer-scale layers. These materials store chemical energy in a manner similar to conventional explosives and remain inert until activated. (See *S&TR*, November/December 2008, pp. 10–16.)

Testing Explosives

Explosives tests at HEAF are conducted in one of seven indoor firing tanks. The tanks range from a 76-centimeter-diameter tank rated for 7.5 grams of TNT-equivalent explosives to a 4.9-meter-diameter tank rated for 10 kilograms. The facility also has a capability for shock compression experiments using large gas guns. For high-velocity impact studies, a 100-millimeter-diameter single-stage gas gun is fired into a specially designed tank. The gun uses several kilograms of propellant and achieves projectile velocities up to 2,500 meters per second.

A two-stage gun at HEAF fires smaller-diameter projectiles to velocities of about 8,000 meters per second. The two-stage gun is a companion to one at the Joint Actinide Shock Physics Experimental Research Facility at the Nevada National Security Site, where actinide research is conducted. Other resources include a range of guns for testing small-caliber ammunition and a microdetonics laboratory for studies at the millimeter to micrometer scale.

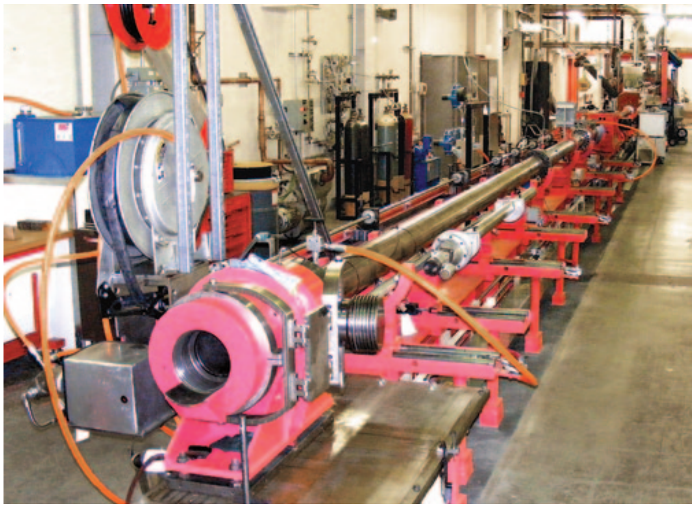
HEAF laboratories are used to characterize energetic materials for their safety, sensitivity, and mechanical and thermal stability. The detonation products of these energetic materials are determined as well. Tests are thoroughly instrumented with high-speed diagnostics including x-ray radiography, x-ray computed tomography, high-speed photography, and laser velocimetry.

"We run experiments with high-fidelity diagnostics that collect a large amount of precise data," says Maienschein. "Where we once would run dozens of experiments to obtain the information we wanted, we now need only a few, especially if we use computer simulations to design the initial experiment."

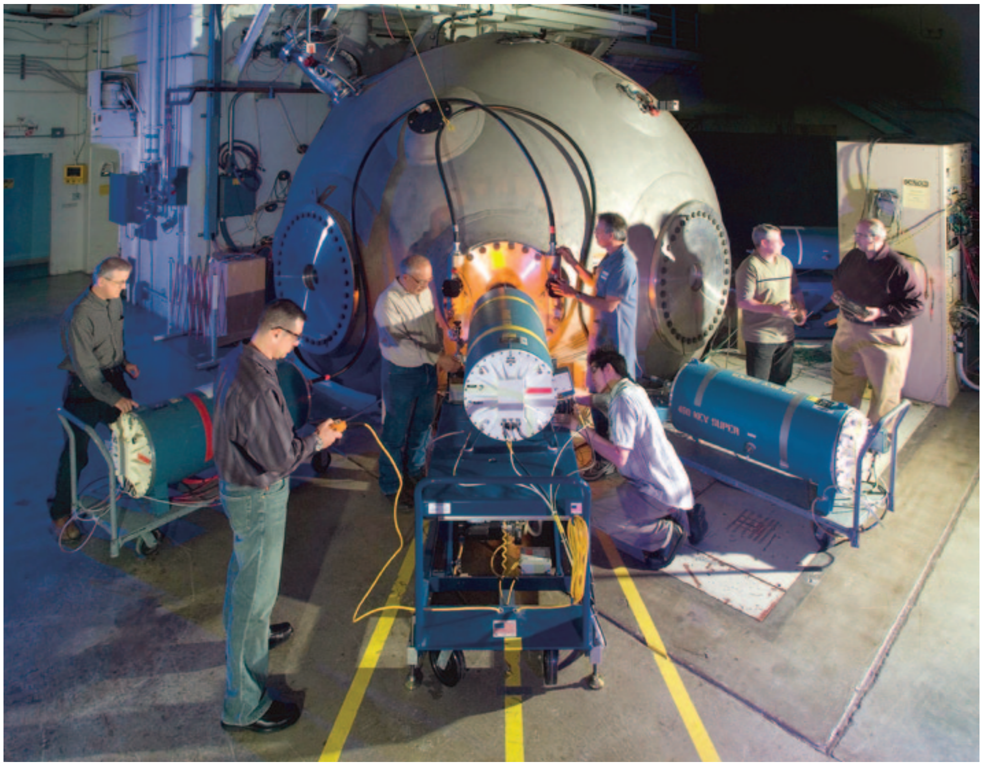
Maienschein cites long-standing efforts to develop ever-more-accurate diagnostics. One of Livermore's most important diagnostic instruments is the photonic Doppler velocimeter (PDV), which uses standard fiber optics and commercial digitizers. Easy to operate and extremely accurate, PDV records continually changing velocities by measuring the Doppler-shifted frequency of light reflected off a surface. (See *S&TR*, July/August 2004, pp. 23–25.)

Site 300 Operations

Energetic material fabrication ranges from the gram-to-kilogram scale at HEAF to hundreds of kilograms at Site 300, 24 kilometers southeast of the Labortory's main site.



In HEAF's two-stage gas gun, the first stage uses gunpowder and a piston to compress a light drive gas, typically hydrogen, to very high pressures. A rupture disk releases the drive gas into a smaller diameter launch tube, which contains the experimental projectile. The launch tube guides the projectile to the target chamber, which connects to diagnostic instruments outside the chamber.



Explosives tests at HEAF are conducted in one of seven indoor firing tanks. Here, HEAF technicians and engineers ready a test at the spherical tank rated for a maximum of 10 kilograms of trinitrotoluene- (TNT-) equivalent explosives. The blue cylinders arrayed around the tank form the Hydra x-ray diagnostic, which records a multi-image time sequence of each shot.

Fabrication activities at Site 300 include large-scale synthesis, formulation, pressing, machining, and assembly. The capability to manufacture large precision melt-cast explosives parts is unique to NNSA and the nation.

The casting of large amounts of high explosives at Site 300 is supervised by formulation chemist Sabrina DePiero and others, who work both at HEAF and at Site 300. Much of the casting work supports counterterrorism programs that test large explosive devices for determining their properties as IEDs and as part of improvised nuclear devices, which would presumably use HE along with some type of nuclear material.

Some "melt castable" explosives, such as Composition B (a mixture of TNT and RDX [1,3,5-trinitro-1,3,5-triazacyclohexane]), are gently heated and poured into molds. A team of chemists, mechanical engineers, and technicians oversees the explosives casting at Site 300's Building 827 complex, which includes a control room as well as three earth-covered cells for explosives processing. "Casting Composition B in a large kettle is similar to making caramel candy," says Site 300 Manager John E. Scott. Once melted, the explosive is poured into a mold, slow-cooled by a water bath, and later machined to the precise shape needed to accommodate instruments.

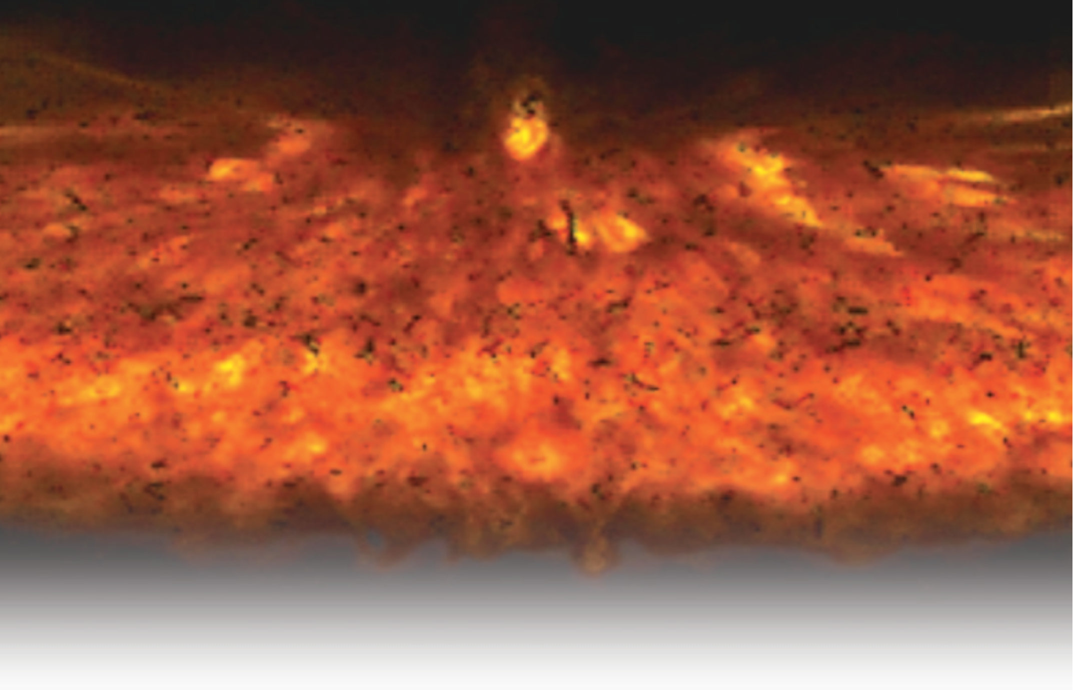
Other types of explosives are pressed into rough shapes, machined into precise shapes, and fitted with a variety of diagnostic sensors. With still other explosives, such as LX-20, binders are added to HMX (tetranitro tetraazacyclooctane), and mixing is done remotely under closed circuit cameras. The mixture can then be extruded in molds, where it cures into a solid.

Up to 45 kilograms of energetic materials are detonated at one outdoor facility, where detonation characteristics are examined for myriad applications and programs. Up to 60 kilograms of energetic materials can be detonated inside the 2,600-square-meter Contained Firing Facility (CFF), the largest indoor firing facility in the world. Energetic parts heavier than 60 kilograms are transported to the Nevada National Security Site or a Department of Defense site for testing.

CFF offers the nation's most extensive suite of diagnostic equipment for studying the detonation of explosives. Most experiments conducted at CFF support the Laboratory's stockpile stewardship efforts. The facility's flash x-ray machine, the only wide-angle penetrating radiography accelerator in the NNSA complex, captures the density and symmetry of compressed metals in 65-billionths of a second. Ultrahigh-speed rotating mirror cameras capture up to 160 consecutive frames of images at 3 million frames per second, forming a movielike record of an experiment. Testing capabilities are complementary to those at the Dual-Axis Radiographic Hydrodynamic Test Facility at Los Alamos National Laboratory, according to Jack Lowry, who leads explosives firing operations at CFF.

EMC scientists with forensic training also support the Forensic Receival Facility at Site 300. The facility is operated by

High-speed (30,000 frames per second) video captures the several-meters-wide dispersion of a thermite reaction inside HEAF's 10-kilogram spherical tank. Thermites are combinations of a metal powder and a metal oxidant. This frame occurs 1.29 milliseconds following the onset of the reaction.



The casting of large explosive charges is conducted at Site 300. For the explosive Composition B, dry chips are first placed into a melt-cast kettle and then poured into a hemispherical mold assembly and cooled. (left) Chemistry technician Aaron Fontes (shown left) and supervisor Patrick Gallagher remove the upper mold assembly, exposing the cooled, inverted hemisphere. The part's core does not contain any explosive. (below) Posing by the cooled hemispherical part are (from left) Fontes, Gallagher, formulation chemist Sabrina DePiero, engineering technicians Adriano Salamanca and George Governo, and engineer Doug Dobie. The part was then machined, joined to its twin, and transported to the Nevada National Security Site for testing.

Livermore's Forensic Science Center (FSC), where experts determine the composition and often the source of minute samples of evidence to counter terrorism, aid domestic law enforcement, and verify compliance with international treaties.

The Forensic Receival Facility is designed to ensure chain of custody of evidentiary materials if a terrorist on U.S. soil detonates an explosive. At the FBI's request, explosives involved in a terrorist event would be received, sampled, and temporarily stored at the facility. A climate- and contamination-controlled, air-filtered transportainer is dedicated to processing HE-contaminated evidence delivered to the facility following such an event. Samples would eventually be transported by a specialized van to Livermore for detailed analysis at the FSC analytical laboratories and HEAF. An FBI-led exercise in 2009 demonstrated the utility of the Forensic Receival Facility, if it should be required.

Worldwide Influence

Although much of the energetic materials research must remain classified, Livermore researchers publish 40 to 50 journal articles each year in leading international science journals. Simpson is the U.S. editor, and Livermore chemist Richard Gee is the U.S. associate editor of *Propellants, Explosives, Pyrotechnics*, which is published in Germany by Wiley-VCH. In addition, the Laboratory cosponsors the International Detonation Symposium Series, which began in 1951.

Such international exposure and academic collaboration help strengthen the expertise and influence of EMC researchers, notes Maienschein. From precise explosive devices that destroy terrorists (but not close-by civilians), to the devastating explosive power of highly penetrating bombs, to remarkably insensitive formulations in nuclear weapons, energetic materials are the focus of myriad innovative research efforts at the Laboratory.

—Arnie Heller

Key Words: ALE3D, CHEETAH, Composition B, Contained Firing Facility (CFF), Energetic Materials Center (EMC), flash x ray, Forensic Receival Facility, high explosive (HE), High Explosives Applications Facility (HEAF), improvised explosive device (IED), insensitive high explosive (IHE), National Explosives Engineering Sciences Security Center, photonic Doppler velocimeter (PDV), Site 300, Stockpile Stewardship Program, tetranitro tetraazacyclooctane (HMX), 1,3,5-triamino-2,4,6-trinitrobenzene (TATB), 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX), trinitrotoluene (TNT).

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